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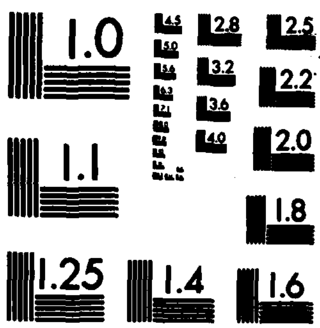

MICROCOPY RESOLUTION TEST CHART
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The objective of the research summerized here was to determine the stress dependence of the chemical potential of atoms chemisorbed to metal surfaces.

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Before going into detail, let us give the reader the main highlights of the accomplishments thus far.

Prompted by our work on the physics and chemistry of surfaces, we have developed a new band theory of crytalline solids that is general, i.e., can be applied to all crystalline solids. This work was presented at the 1984 International Conference of Quantum Chemistry (Saibel Symposium) and was so well received that the internationally renowned physicist and organizer of the conference, Professor Per Olov Lowdin stated, and we quote his exact words:

"We have been waiting for this for twenty years. You have done it and it is elegant".

We are now in the process of improving the numerical computational capacity of our software and computer system so that we can then go into the next phase: the introduction of a "surface" into the theory to get back to the phenomenon we started from, namely chemisorption on solid crystalline solids under stress.

Let us now go into the second highlight of our investigation. Again this phase of our work was prompted by the physical reality that we have to deal with the thermodynamics of the adsorption process--better stated, the statistical mechanics of the formation of patterns of adsorption of atoms on surface sites. Because these adsorbed atoms interact with each other and form "phases" on the surface (different patterns, depending on temperature), there is the problem of predicting these patterns from theory. Because those transitions are taking place, we are to deal with nonequilibrium statistical physics.

Preliminary to this second phase we applied the theory of "Renormalization Group" to quantum optics, to test our ideas and become proficient in this field. We developed the first application of this theory to Quantum Optics, and the work was recently presented at the Stiges International Conference on Statistical Physics and was well received. We are developing further tools of this theory so as to get back to the original problem of dealing with phase transformations of adsorbed species on surfaces under stress applied to the solid substrate.

The third highlight of our work stems from the following practical question: How are we going to detect experimentally changes of adsorptive behavior under stress? We provided a direct answer to this question by coming up with a new method of detection of these changes that uses Raman Scattering. We showed, for the first time, quantitatively, that radiation that is Raman scattered by the adsorbed species will be shifted in frequency due to the stresses in the solid substrate. This new "stress activated Raman Scattering" (STARS) was also well received by the scientific-engineering community. Interest was shown to carry out the experiments suggested in our paper and we hope that this phase will also come to fruition.

We must now emphasize that before we delved into the more complex theoretical work just outlined, we carried out several benchmark theoretical investigations on our chemostress effect. These papers were well received by both scientific and engineering communities as evidenced by reprint requests that we received from almost all countries in Europe, several major countries in Asia, Canada, Africa and the U.S., and we gave many invited papers at international conferences here and abroad.

In brief, we show that stresses can change adsorptive and diffusive behavior leading to stress-corrosion cracking, anomalous adsorptive behavior that is environment dependent (such as wetness) called the Rebinder Effect, and elucidated mechanisms of wear. We were able to single out a fundamental mechanism for the initiation of a crack, its precursor. We showed that the concept of a chemical potential first defined by Gibbs could be correctly extended to quantitatively calculate this chemostress effect at three levels of detail: 1) statistical thermodynamics that also used empirical results, 2) quantum statistical mechanics that is semiclassical in that we used Maxwell's equation for dielectric response, 3) fully quantized model Hamiltonian level that uses Green's functions.

All three methods showed the existence of such an effect.

Armed with these findings we tried to see how we could account for observed anomalous adsorptive and diffusive processes that arise in wear, crack propagation, stress corrosion and hardness measurements (Rebinder Effect). We were able to explain for the first time in detail the origin of the elusive but measurable "zeta potential" associated with environment dependent hardness measurements.

Having thus grasped the real physical processes that were operative we could embark on a more fundamental first principles microscopic theory, namely calculating the exact energy spectra of solids in contact with adsorbed species. This was necessary since "chemi sorption, as opposed to physi sorption, requires taking into account of the changes in electronic orbitals of the adatom as these orbitals do penetrate into the solid substrate or repel them, and become localized or delocalized (in the Anderson sense).

We have given more technical details of the rationale in our proposal 21178-PH.

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Mikael Ciftan

MIKAEL CIFTAN

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